

epi-«gamma»-Eudesmol

Other names:	7-epi-«gamma»-Eudesmol
Inchi:	InChI=1S/C15H26O/c1-11-6-5-8-15(4)9-7-12(10-13(11)15)14(2,3)16/h12,16H,5-10H2,1-4H
InchiKey:	WMOPMQRJLLIEJV-DOMZBBRYSA-N
Formula:	C15H26O
SMILES:	CC1=C2CC(C(C)(C)O)CCC2(C)CCC1
Mol. weight [g/mol]:	222.37

Physical Properties

Property code	Value	Unit	Source
gf	19.75	kJ/mol	Joback Method
hf	-342.87	kJ/mol	Joback Method
hfus	13.30	kJ/mol	Joback Method
hvap	65.35	kJ/mol	Joback Method
log10ws	-4.64		Crippen Method
logp	4.064		Crippen Method
mcvol	202.060	ml/mol	McGowan Method
pc	2191.78	kPa	Joback Method
rinpol	1591.00		NIST Webbook
rinpol	1610.00		NIST Webbook
rinpol	1610.00		NIST Webbook
rinpol	1591.00		NIST Webbook
rinpol	1622.00		NIST Webbook
rinpol	1603.00		NIST Webbook
rinpol	1609.00		NIST Webbook
rinpol	1619.00		NIST Webbook
rinpol	1609.00		NIST Webbook
rinpol	1619.00		NIST Webbook
ripol	2099.00		NIST Webbook
ripol	2076.00		NIST Webbook
ripol	2103.00		NIST Webbook
ripol	2137.00		NIST Webbook
ripol	2095.00		NIST Webbook
ripol	2076.00		NIST Webbook
tb	671.47	K	Joback Method
tc	884.60	K	Joback Method
tf	393.55	K	Joback Method
vc	0.750	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	596.14	J/mol×K	671.47	Joback Method
cpg	615.41	J/mol×K	706.99	Joback Method
cpg	633.66	J/mol×K	742.51	Joback Method
cpg	651.05	J/mol×K	778.04	Joback Method
cpg	667.73	J/mol×K	813.56	Joback Method
cpg	683.86	J/mol×K	849.08	Joback Method
cpg	699.60	J/mol×K	884.60	Joback Method

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R203953&Units=SI

Legend

cpg:	Ideal gas heat capacity
gf:	Standard Gibbs free energy of formation
hf:	Enthalpy of formation at standard conditions
hfus:	Enthalpy of fusion at standard conditions
hvap:	Enthalpy of vaporization at standard conditions
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
pc:	Critical Pressure
rinpol:	Non-polar retention indices
ripol:	Polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature

tf: Normal melting (fusion) point

vc: Critical Volume

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